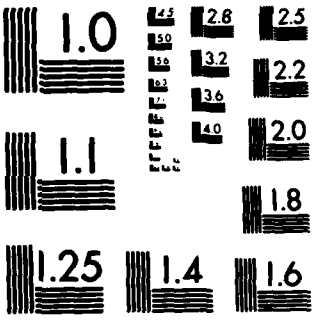
AD-A148 722 OPTIMISATION OF THE THERMOELECTRIC FIGURE OF MERIT IN FINE GRAINED SEMICO..(U) UNIVERSITY OF WALES INST OF SCIENCE AND TECHNOLOGY CARDIFF DE.. D M ROWE ET AL. 1/1

UNCLASSIFIED DEC 82 DAJA37-82-C-0016 F/G 20/3 NL



OPTIMISATION OF THE THERMOELECTRIC FIGURE OF MERIT IN FINE GRAINED SEMICONDUCTOR MATERIALS BASED UPON LEAD TELLURIDE

D M Rowe and C M Bhandari

Department of Physics, Electronics and Electrical Engineering,
University of Wales Institute of Science & Technology,
King Edward VII Avenue,
Cardiff CF1 3NU, U.K.

1st Periodic Report October 1982 - December 1982

The Research reported in this document has been made possible through the support and sponsorship of the United States Government through its European Research Office of the U.S. Army. This report is intended only for the internal management of the Contractor and the U.S. Government.

Contract Number DAJ37-82-00016

OPTIMISATION OF THE THERMOELECTRIC FIGURE OF MERIT IN FINE GRAINED SEMICONDUCTOR MATERIALS BASED UPON LEAD TELLURIDE

I. Work Undertaken

The programme of work follows that set out in the initial report and it is proceeding on schedule. A model has been formulated for the lead telluride system and the effect of phonon-grain boundary scattering, doping and alloying on the lattice thermal conductivity of lead telluride investigated. The preliminary results of our work are embodied in the attached paper. The paper entitled "The Effect of Phonon-Grain Boundary Scattering, Doping and Alloying on the Lattice Thermal Conductivity of Lead Telluride" has been submitted for publication in Journal of Physics D. The main conclusion we reach is that in moderately doped materials with a grain size of 1 μm, the reduction in lattice thermal conductivity would be in the range 4 to 6 per cent for unalloyed lead telluride and 11 to 13 per cent for highly disorded alloys.

II. Future Programme of Work

The next step is to investigate the material figure of merit Z. This is a difficult undertaking as it involves the separation of the lattice and electronic contributions of the thermal conductivity. Our literature survey has revealed that there is very little European/USA published information on the value and behaviour of the Lorenz number for lead telluride materials - what information there is is of Soviet origin and indicates a peculiar behaviour. Correspondence with a number of authors of papers on thermoelectric transport theory has shed little light on the problem and this is a topic which we are currently investigating.

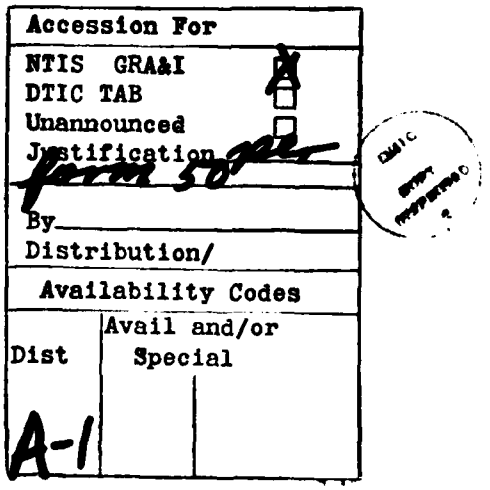
III. Availability of Lead Telluride Materials

In order to fit our theoretical model to actual materials experimental data is required. As this data is not available in the literature we had planned to make a number of measurements of the thermal and electrical properties of lead telluride type materials. Following a communication with Dr Guido Guazzoni (Fort Monmouth, USA)

to "Global Power Systems" (Alberta, Canada) - the most recent dated 25th November 1982.

IV. Continuation of Project

By the end of October 1983 we will have completed our calculations of and will be in a position to start relating our model to actual materials with the view to providing advice on which combination of doping level, grain size and alloying is likely in practice to give the best thermo-electric performance. In order to plan our future programme of work could some indication be given of the likelihood of continuing the project beyond October 1983.



Paper submitted for publication in J Phys D.

The Effect of Phonon-Grain Boundary Scattering, Doping and Alloying on the Lattice Thermal Conductivity of Lead Telluride

C M Bhandari* and D M Rowe

Department of Physics, Electronics and Electrical Engineering
UWIST, King Edward VII Avenue, Cardiff CF1 3NU

Abstract

The lattice thermal conductivity of lead telluride has been investigated theoretically as a function of grain size, level of doping and alloying. Although there is some difficulty in making predictions of the precise dependence of the lattice thermal conductivity on these parameters, it is possible to indicate the range over which the results may vary. It is concluded that for moderately doped material having a grain size of 1μm the reduction in lattice thermal conductivity would lie in the range 4 - 6 percent for unalloyed lead telluride and 11-13 percent for highly disordered alloys.

It has been reported that phonon-grain boundary scattering has a significant effect in reducing the lattice thermal conductivity of silicon germanium alloys; an established semiconductor material for high temperature thermoelectric application. (Goldsmid and Penn 1968, Parrott 1969, Bhandari and Rowe 1977, 1978, Rowe, Shukla and Savvides 1981). This pheonomenon does not appear to be accompanied by a deterioration in the performance of the other parameters which occur in the materials thermoelectric figure of merit. Consequently small grain size silicon germanium alloys should exhibit a higher figure of merit than comparable "single crystal" or large grain size material (Rowe and Shukla 1981). Although scattering of phonons by grain boundaries is particularly favoured in silicon germanium alloys because the large difference in atomic masses of the constituent atoms gives rise to substantial alloy disorder scattering, this phenomenon will also manifest itself in other thermoelectric materials.

*On leave from the University of Allahabad India

Thermocouples fabricated from lead telluride and its isomorphous alloys are employed in fossil fueled thermoelectric generators used in a number of US military applications. (Guazzoni and Swaylik 1982). Any reduction in the thermal conductivity of lead telluride and consequent improvement in the devices thermoelectric conversion efficiency will be reflected in a saving of fuel - an important factor when the generator is deployed in a tactical situation. In this brief note the results of a preliminary theoretical analysis of the lattice thermal conductivity of lead telluride as a function of doping, grain size, and alloying is reported.

The model adopted and the notation used has been described in a previous paper (Parrott 1969). It is suffice to state that in general the lattice thermal conductivity K can be expressed in terms of parameters A, B and C. A depends upon disorder (alloying), B is a measure of the strength of phonon-electron/hole coupling (doping). C is usually expressed in terms of a parameter D, which is inversely proportional to the grain size L, and they are related by D = CT where T is the temperature. A = 0 corresponds to unalloyed material with no disorder present, B = 0 corresponds to undoped and C = 0 to single crystal material. In general, $K(A,B,C = 0) = K_{single}$ represents the lattice thermal conductivity of a doped single crystal alloy. A more rigorous analysis would include information about the phonon dispersion relations (Bhandari and Rowe 1977) and this will be discussed in a future communication.

Plots of K/K_{single} at room temperature for unalloyed lead telluride (A = 0) and highly disordered alloys of lead telluride (A = 5) are displayed in figures 1 and 2 as functions of grain size and level of doping. Although there is some difficulty in making an accurate prediction of the dependence of the lattice thermal conductivity on the various parameters because of a lack of experimental data and the uncertainty in the appropriate value for k_o, it is possible to estimate the range over which the results will vary. In undoped lead telluride, the reduction in lattice

thermal conductivity ie $(1-K/K_{single})x100$ for a grain size of 1μm is around 6 percent. For doped lead telluride (10^{24} -10^{25} m^{-3}) this reduction may decrease to 5%. However, in alloys of lead telluride with components differing significantly in molecular weight, the reduction could be as large as 13 percent. We conclude that for moderately doped materials the reduction in lattice thermal conductivity could be in the range 4 - 6 percent - for unalloyedlead telluride and 11 to 13 percent for highly disordered alloys.

Acknowledgements

The United States Army through its' European Research Offices is acknowledged for sponsoring this research under contract No DAJA37-82-C-0116.

References

Bhandari C M And Rowe D M, 1977. J Phys D. App Phys 10, L59 and L247.

- 1978 J Phys C, Solid State Phys. 11. 1787.

Goldsmid H J and Penn A W, 1968, Phys Lett. 27A, 523.

Guazzoni G and Swaylik W, 1982, Proceedings of Fourth International Conference on Thermoelectric Energy Conversion, University of Texas at Arlington, March 10-12. p1.

Parrott J E, 1969, J Phys C. Solid State Phys 2, 147.

Rowe D M, Shukla V S and Savvides N, 1981, Nature Vol 290 No 5809 p765.

Rowe D M and Shukla V S, 1981, J Appl Phys, 52, 12, 8421.

Figure 1 Plot of K/K_{single} for unalloyed lead telluride at 300K as a function of grain size and level of doping

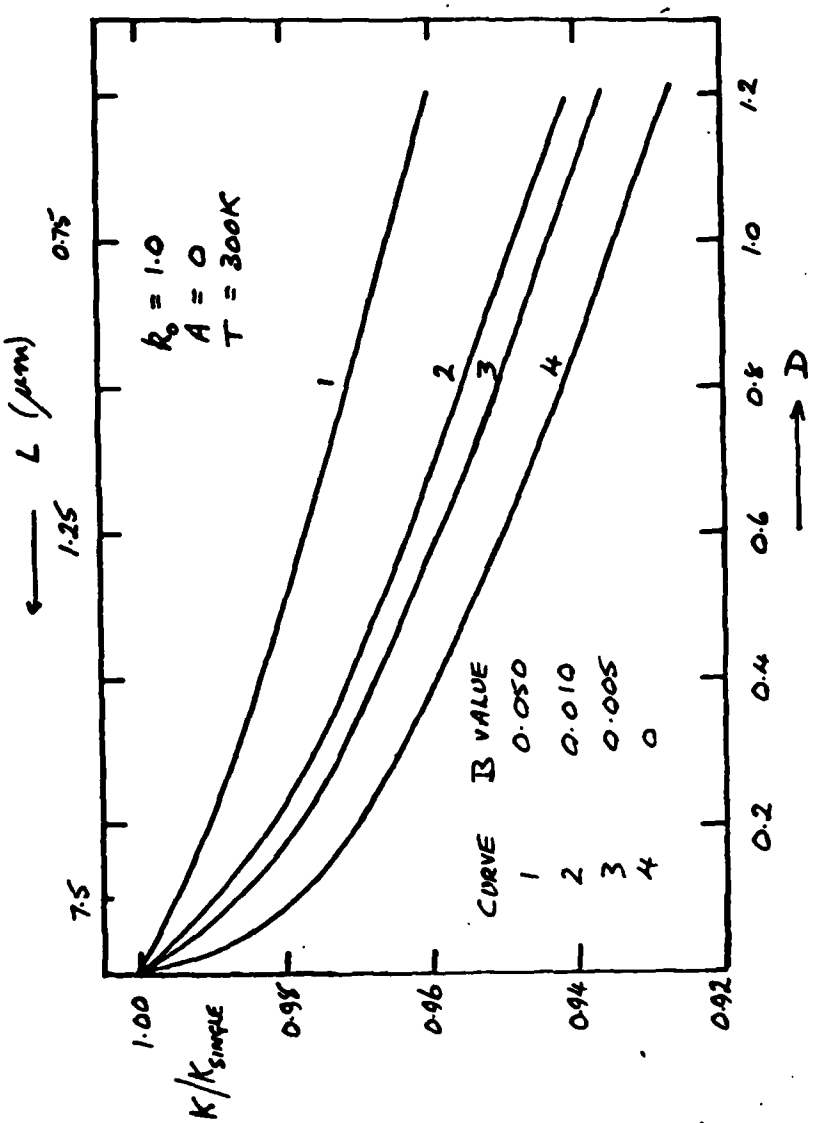
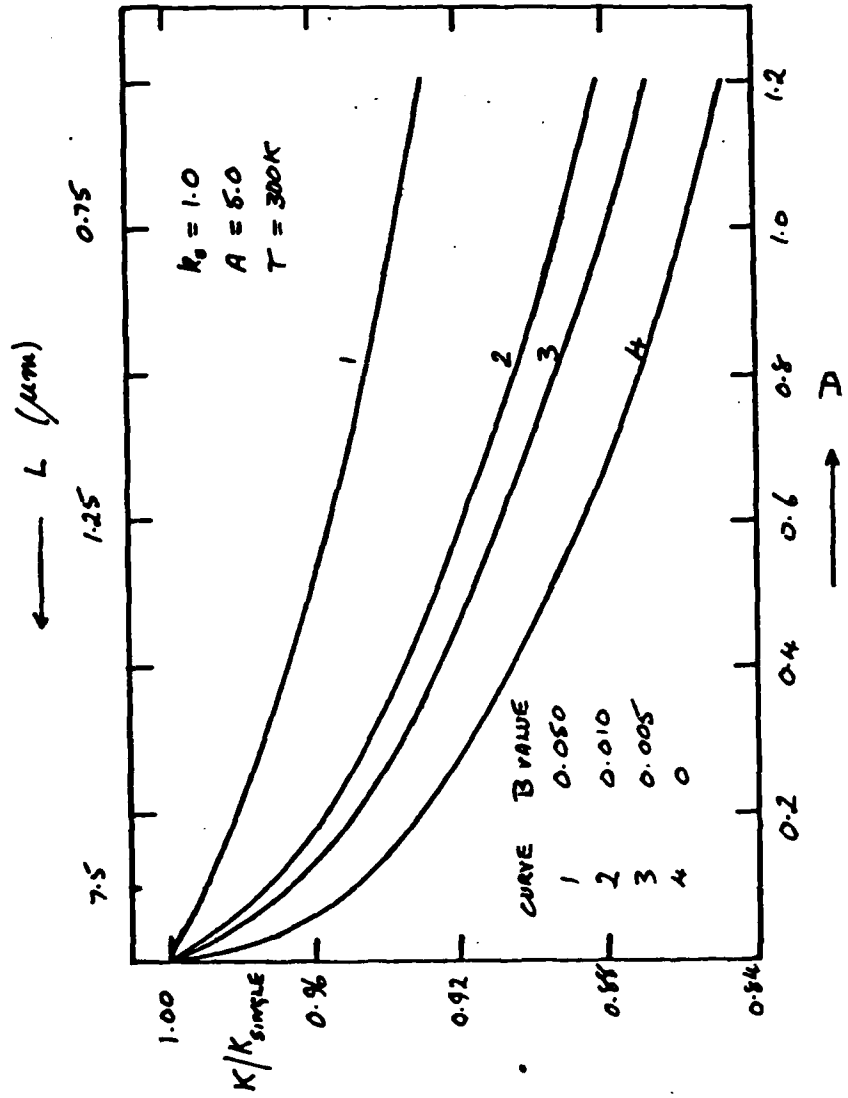


Figure 2 Plot of K/K_{single} for highly disordered alloys of lead telluride at 300K as a function of grain size and level of doping



END

FILMED

1-85

DTIC